On graphlike k-dissimilarity vectors

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Abstract

Let $\mathcal{G} = (G, w)$ be a positive-weighted simple finite graph, that is, let G be a simple finite graph endowed with a function w from the set of the edges of G to the set of the positive real numbers. For any subgraph G' of G, we define $w(G')$ to be the sum of the weights of the edges of G'. For any $i_1, ..., i_k$ vertices of G, let $D_{\{i_1,....i_k\}}(\mathcal{G})$ be the minimum of the weights of the subgraphs of G connecting $i_1, ..., i_k$. The $D_{\{i_1,....i_k\}}(\mathcal{G})$ are called k-weights of $\mathcal{G}$.

Given a family of positive real numbers parametrized by the k-subsets of $\{1, ..., n\}$, $\{D_I\}_{I \in \binom{\{1,...,n\}}{k}}$, we can wonder when there exist a weighted graph $\mathcal{G}$ (or a weighted tree) and an n-subset $\{1, ..., n\}$ of the set of its vertices such that $D_I(\mathcal{G}) = D_I$ for any $I \in \binom{\{1,...,n\}}{k}$. In this paper we study this problem in the case $k = n - 1$.

1 Introduction

For any graph G, let $E(G)$, $V(G)$ and $L(G)$ be respectively the set of the edges, the set of the vertices and the set of the leaves of G. A **weighted graph** $\mathcal{G} = (G, w)$ is a graph G endowed with a function $w : E(G) \to \mathbb{R}$. For any edge e, the real number $w(e)$ is called the weight of the edge. If all the weights are nonnegative (resp. positive), we say that the graph is **nonnegative-weighted** (resp. **positive-weighted**), if all the weights are nonnegative and the ones of the internal edges are positive, we say that the graph is **internal-positive-weighted**. Throughout the paper we will consider only simple finite graphs.

For any subgraph G' of G, we define $w(G')$ to be the sum of the weights of the edges of G'.

Definition 1. *Let $\mathcal{G} = (G, w)$ be a nonnegative-weighted graph. For any distinct $i_1, ..., i_k \in V(G)$, we define*

$$D_{\{i_1,....,i_k\}}(\mathcal{G}) = min\{w(R) |\ R \text{ a connected subgraph of } G \text{ such that } V(R) \ni i_1, ..., i_k\}.$$

*More simply, we denote $D_{\{i_1,....,i_k\}}(\mathcal{G})$ by $D_{i_1,....,i_k}(\mathcal{G})$ for any order of $i_1, ..., i_k$. We call the $D_{i_1,....,i_k}(\mathcal{G})$ the k-**weights** of $\mathcal{G}$ and we call a k-weight of $\mathcal{G}$ for some k a **multiweight** of $\mathcal{G}$.*

If S is a subset of $V(G)$ and we order in some way the k-subsets of S (for instance, we order S in some way and then we order the k-subsets of S in the lexicographic order with respect

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the order of S), the k-weights with this order give a vector in $\mathbb{R}^{\binom{\sharp S}{k}}$. This vector is called **k-dissimilarity vector** of $(\mathcal{G}, S)$. Equivalently, if we don't fix any order, we can speak of the **family of the k-weights** of $(\mathcal{G}, S)$.

We can wonder when a family of real numbers is the family of the k-weights of some weighted graph and of some subset of the set of its vertices. If S is a finite set, $k \in \mathbb{N}$ and $k < \sharp S$, we say that a family of positive real numbers $\{D_I\}_{I \in \binom{S}{k}}$ is **p-graphlike** (resp. nn-graphlike, ip-graphlike)) if there exist a positive-weighted (resp. nonnegative-weighted, internal-positive-weighted) graph $\mathcal{G} = (G, w)$ and a subset S of the set of its vertices such that $D_I(\mathcal{G}) = D_I$ for any I k-subset of S. If the graph is a positive-weighted tree, we say that the family is **p-treelike**; if the graph is a positive-weighted tree and $S \subset L(G)$, we say that the family is **p-l-treelike** (and analogously for nonnegative-weighted or positive-internal-weighted trees).

The first contribute to the characterization of the graphlike families of numbers is due to Hakimi and Yau; in 1965, they observed that a family of positive real numbers $\{D_I\}_{\{I\} \in \binom{\{1,\dots,n\}}{2}}$ is p-graphlike if and only if the D_I satisfy the triangle inequalities.

In the same years, also a criterion for a metric on a finite set to be nn-treelike was established, see [B], [SimP], [St]:

Theorem 2. *Let $\{D_I\}_{I \in \binom{\{1,\dots,n\}}{2}}$ be a set of positive real numbers satisfying the triangle inequalities. It is p-treelike (or nn-l-treelike) if and only if, for all $i, j, k, h \in \{1, ..., n\}$, the maximum of*

$$\{D_{i,j} + D_{k,h}, D_{i,k} + D_{j,h}, D_{i,h} + D_{k,j}\}$$

is attained at least twice.

In terms of tropical geometry, the theorem above can be formulated by saying that the set of the 2-dissimilarity vectors of weighted trees with n leaves and such that the internal edges have negative weights is the tropical Grassmanian $\mathcal{G}_{2,n}$ (see [S-S]).

For $k = 2$ also the case of not necessarily nonnegative weights has been studied. For any weighted graph $\mathcal{G} = (G, w)$ and for any $i, j \in V(G)$, we define $D_{i,j}(\mathcal{G})$ to be the minimum of $w(p)$ for p a simple path joining i and j. Again, we call such numbers "2-weights". In 1972 Hakimi and Patrinos proved that a family of real numbers $\{D_I\}_{\{I\} \in \binom{\{1,\dots,n\}}{2}}$ is always the family of the 2-weights of some weighted graph and some subset $\{1, ..., n\}$ of its vertices.

In [B-S], Bandelt and Steel proved a result, analogous to Buneman's one, for general weighted trees, precisely they proved that, for any set of real numbers $\{D_I\}_{\{I\} \in \binom{\{1,\dots,n\}}{2}}$, there exists a weighted tree $\mathcal{T}$ with leaves $1, ..., n$ such that $D_I(\mathcal{T}) = D_I$ for any I 2-subset of $\{1, ..., n\}$ if and only if, for any $a, b, c, d \in \{1, ..., n\}$, we have that at least two among $D_{a,b} + D_{c,d}$, $D_{a,c} + D_{b,d}$, $D_{a,d} + D_{b,c}$ are equal.

For higher k the literature is more recent. In 2004, Pachter and Speyer proved the following theorem (see [P-S]).

Theorem 3. ***(Pachter-Speyer)****. Let $k, n \in \mathbb{N}$ with $n \geq 2k - 1$ and $k \geq 3$. A positive-weighted tree $\mathcal{T}$ with leaves $1, ..., n$ and no vertices of degree 2 is determined by the values $D_I(\mathcal{T})$, where I varies in $\binom{\{1,\dots,n\}}{k}$.*

In [H-H-M-S], the authors gave the following characterization of the ip-l-treelike families of positive real numbers:

Theorem 4. ***(Herrmann, Huber, Moulton, Spillner)***. *If $n \geq 2k$, a family of positive real numbers $\{D_I\}_{I \in \binom{\{1,...,n\}}{k}}$ is ip-l-treelike if and only if the restriction to every $2k$-subset of $\{1,...,n\}$ is ip-l-treelike.*

Besides they studied when a family of positive real numbers is ip-l-treelike in the case $k = 3$.

Finally, in [Ru1] and [Ru2], for any weighted tree $\mathcal{T}$, for $k \geq 2$ and for any distinct leaves $i_1, ..., i_k$, the author defines $D_{i_1,....,i_k}(\mathcal{T})$ to be the sum of the lengths of the edges of the minimal subtree joining i_1,....,i_k and gives an inductive characterization of the families of real numbers indexed by the subsets of $\{1, ..., n\}$ of cardinality greater or equal than 2, that are the families of the multiweights of a tree with n leaves and the set of its leaves.

Let $n, k \in \mathbb{N}$ with $n > k$. In this paper we study the problem of the characterization of the families of positive real numbers, indexed by the k-subsets of an n-set, that are p-graphlike. As we have already said, the case $k = 2$ has already been studied by Hakimi and Yau. Here we examine the case $k = n - 1$, both for trees (Section 3) and graphs (Section 4), see Theorems 9, 10, 11 and 13.

2 Notation and a first remark

Notation 5. • *Let $\mathbb{R}_+ = \{x \in \mathbb{R} | \ x > 0\}$.*

• *For any $n \in \mathbb{N}$ with $n \geq 1$, let $[n] = \{1, ..., n\}$.*

• *For any set S and $k \in \mathbb{N}$, let $\binom{S}{k}$ be the set of the k-subsets of S.*

• *Throughout the paper, we will consider only simple finite graphs. For any $v, v' \in V(G)$, let $e(v, v')$ denote the edge joining v and v'.*

• *For simplicity, the vertices of graphs will be often named with natural numbers. In the figures the names of the vertices will be written in bold calligrahic in order to avoid confusion with the weights.*

Definition 6. *Let $\mathcal{G} = (G, w)$ be a positive-weighted graph. We say that a connected subgraph of G, R, realizes $D_{i_1,....,i_k}(\mathcal{G})$, or it is a* ***subgraph realizing*** *$D_{i_1,....,i_k}(\mathcal{G})$ if $i_1, ..., i_k$ are vertices of R and $w(R) = D_{i_1,....,i_k}(\mathcal{G})$. Observe that it is necessarily a tree, so we will call it also* ***subtree realizing*** *$D_{i_1,....,i_k}(\mathcal{G})$.*

Let S be a finite set. If D_I for $I \in \binom{S}{k}$ are positive real numbers and there exist a nonnegative weighted graph $\mathcal{G} = (G, w)$ and a subset S of $V(G)$, such that $D_I(\mathcal{G}) = D_I$ for any $I \in \binom{S}{k}$, then we say that $(\mathcal{G}, S)$ realizes the family $\{D_I\}_{I \in \binom{S}{k}}$ and, following [H-Y], we call the vertices in S ***external vertices*** *and the other vertices* ***internal vertices****.*

Remark 7. *Let $\mathcal{G} = (G, w)$ be a positive-weighted graph; then, for any $I, J, K \subset V(G)$ with $J \cap K \neq \emptyset$ and $J \cup K \supset I$, we have the "triangle inequality"*

$$D_I(\mathcal{G}) \leq D_J(\mathcal{G}) + D_K(\mathcal{G}). \qquad (1)$$

Proof. Let G' and G'' be two subgraphs of G realizing respectively $D_J(\mathcal{G})$ and $D_K(\mathcal{G})$: the union of these subgraphs is a connected subgraph, G''', whose set of vertices contain J and K and then I. So we have:

$$D_I(\mathcal{G}) \leq w(G''') \leq w(G') + w(G'') = D_J(\mathcal{G}) + D_K(\mathcal{G}).$$

□

3 $(n-1)$-dissimilarity vectors of trees with n vertices

In this section we want to examine when a family of positive real numbers $\{D_I\}_{I \in \binom{[n]}{n-1}}$ is treelike.

Notation 8. *Let $n \in \mathbb{N}$, $n \geq 3$. Given a family of real numbers $\{D_I\}_{I \in \binom{[n]}{n-1}}$, we denote $D_{1,\ldots,\hat{i},\ldots,n}$ by $D_{\hat{i}}$ for any $i \in [n]$.*

Theorem 9. *Let $n \in \mathbb{N}$, $n \geq 3$ and let $\{D_I\}_{I \in \binom{[n]}{n-1}}$ be a family of positive real numbers.*

(a) There exists a positive-weighted tree $\mathcal{T} = (T, w)$ with at least n vertices*, $1, \ldots, n$, and such that $D_{\hat{i}}(\mathcal{T}) = D_{\hat{i}}$ for any $i = 1, \ldots, n$ if and only if*

$$(n-2) D_{\hat{i}} \leq \sum_{j \in [n]-\{i\}} D_{\hat{j}} \tag{2}$$

for any $i \in [n]$ and at most one of the inequalities (2) is an equality.

(b) There exists a positive-weighted tree $\mathcal{T} = (T, w)$ with at least n leaves*, $1, \ldots, n$, and such that $D_{\hat{i}}(\mathcal{T}) = D_{\hat{i}}$ for any $i \in [n]$ if and only if*

$$(n-2) D_{\hat{i}} < \sum_{j \in [n]-\{i\}} D_{\hat{j}} \tag{3}$$

for any $i \in [n]$.

Proof. (a) $\Rightarrow$ Let $\mathcal{T} = (T, w)$ be a positive weighted tree and let $[n] \subset V(T)$. We want to show that for any $k \in [n]$

$$(n-2) D_{\hat{k}}(\mathcal{T}) \leq \sum_{j \in [n]-\{k\}} D_{\hat{j}}(\mathcal{T}). \tag{4}$$

Let $G_{1,\ldots,n}$ be a subtree of T realizing $D_{1,\ldots,n}(\mathcal{T})$; obviously it is a tree with set of leaves contained in $[n]$. Let $G_{\hat{k}}$ be a subtree of T realizing $D_{\hat{k}}(\mathcal{T})$; obviously it is a tree with set of leaves contained in $\{1, \ldots, \hat{k}, \ldots, n\}$. Observe that $G_{\hat{k}}$ is a subgraph of $G_{1,\ldots,n}$ (in fact, for every $r, s \in \{1, \ldots, \hat{k}, \ldots, n\}$, the path between r and s in $G_{\hat{k}}$ must coincide with the path between r and s in $G_{1,\ldots,n}$, since T is a tree). For every $k = 1, \ldots, n$, let a_k be the weight of the subgraph $G_{1,\ldots,n} - G_{\hat{k}}$. The inequality (4) becomes

$$(n-2)(D_{1,\ldots,n}(\mathcal{T}) - a_k) \leq \sum_{j \in [n]-\{k\}} (D_{1,\ldots,n}(\mathcal{T}) - a_j),$$

which is equivalent to

$$\sum_{j \in [n]-\{k\}} a_j \leq D_{1,\dots,n}(\mathcal{T}) + (n-2)a_k,$$

which is true, since, obviously, $\sum_{j \in [n]-\{k\}} a_j \leq D_{1,\dots,n}(\mathcal{T})$.

Now we want to prove that at most one of the inequalities (2) is an equality. Suppose

$$(n-2)D_{\hat{k}}(\mathcal{T}) = \sum_{j \in [n]-\{k\}} D_{\hat{j}}(\mathcal{T}).$$

Then

$$\sum_{j \in [n]-\{k\}} a_j = D_{1,\dots,n}(\mathcal{T}) + (n-2)a_k.$$

Since $\sum_{j \in [n]-\{k\}} a_j \leq D_{1,\dots,n}(\mathcal{T})$, we get $a_k = 0$ and

$$D_{1,\dots,n}(\mathcal{T}) = \sum_{j \in [n]-\{k\}} a_j.$$

Thus $G_{1,\dots,n}$ is a star tree with leaves $1, ..., \hat{k}, ..., n$ and center k and $a_j = 0$ if and only if $j = k$. It is easy to check that in this case only one of the inequalities (2) is an equality.

$\Leftarrow$ We consider two cases: the case where all the inequalities (2) are strict and the case where exactly one of the inequalities (2) is an equality.

• First let us suppose that all the inequalities (2) are strict. Let $\mathcal{T}$ be the star tree with $[n]$ as set of leaves and center $n+1$ and, for $k = 1, ..., n$, let

$$w(e(n+1,k)) = \frac{\sum_{j \in [n]-\{k\}} D_{\hat{j}} - (n-2)D_{\hat{k}}}{n-1}.$$

For any $k = 1, ..., n$, we have that $D_{\hat{k}}(\mathcal{T})$ is equal to the sum of the weights of all the edges but the edge $e(n+1,k)$. Therefore

$$D_{\hat{k}}(\mathcal{T}) = \frac{1}{n-1}\left[\sum_{h \in [n]-\{k\}} \left(\sum_{j \in [n]-\{h\}} D_{\hat{j}} - (n-2)D_{\hat{h}}\right)\right] =$$

$$= \frac{1}{n-1}\left[\sum_{h \in [n]-\{k\}} \left(\sum_{j \in [n]} D_{\hat{j}} - (n-1)D_{\hat{h}}\right)\right] =$$

$$= \frac{1}{n-1}\left[(n-1)\left(\sum_{j \in [n]} D_{\hat{j}}\right) - (n-1)\left(\sum_{h \in [n]-\{k\}} D_{\hat{h}}\right)\right] = D_{\hat{k}}.$$

• Now let us suppose that exactly one of the inequalities (2) is an equality, precisely

$$(n-2)D_{\hat{r}} = \sum_{j \in [n]-\{r\}} D_{\hat{j}}. \tag{5}$$

Let $\mathcal{T}$ be the star tree with $\{1, ..., \hat{r}, ..., n\}$ as set of leaves and center r and, for $k \in [n] - \{r\}$, let

$$w(e(r,k)) = \frac{\sum_{j\in[n]-\{k\}} D_{\hat{j}} - (n-2)D_{\hat{k}}}{n-1}.$$

We want to show that, for any $k = 1, ..., n$, we have that $D_{\hat{k}}(\mathcal{T}) = D_{\hat{k}}$. Let $k \neq r$. Thus $D_{\hat{k}}(\mathcal{T})$ is equal to the sum of the weights of all the edges but the edge $e(r,k)$. Therefore

$$D_{\hat{k}}(\mathcal{T}) = \frac{1}{n-1}\left[\sum_{h\in[n]-\{r,k\}} \left(\sum_{j\in[n]-\{h\}} D_{\hat{j}} - (n-2)D_{\hat{h}}\right)\right] =$$

$$= \frac{1}{n-1}\left[\sum_{h\in[n]-\{r,k\}} \left(\sum_{j\in[n]} D_{\hat{j}} - (n-1)D_{\hat{h}}\right)\right] =$$

$$= \frac{1}{n-1}\left[(n-2)\left(\sum_{j\in[n]} D_{\hat{j}}\right) \quad - \quad (n-1)\left(\sum_{h\in[n]} D_{\hat{h}} - D_{\hat{r}} - D_{\hat{k}}\right)\right] =$$

$$= \frac{1}{n-1}\left[-\sum_{j\in[n]} D_{\hat{j}} + (n-1)D_{\hat{r}} + (n-1)D_{\hat{k}}\right] = D_{\hat{k}},$$

where the last equality holds because, by (5), we have that $(n-1)D_{\hat{r}} = \sum_{j=1,...,n} D_{\hat{j}}$. Besides, for any $k \neq r$,

$$D_{\hat{r}}(\mathcal{T}) = D_{\hat{k}}(\mathcal{T}) + w(e(r,k)) = D_{\hat{k}} + w(e(r,k)) = D_{\hat{r}},$$

where the last equality holds again by (5).

(b) $\Rightarrow$ We can argue as in the analogous implication in (a). In this case, since $1, ..., n$ are leaves, all the a_i are nonzero, so we get the strict inequalities (3).

$\Leftarrow$ Let $\mathcal{T}$ be the star tree with $\{1, ..., n\}$ as set of leaves and center $n+1$ and, for $k \in [n]$, let

$$w(e(n+1,k)) = \frac{\sum_{j\in[n]-\{k\}} D_{\hat{j}} - (n-2)D_{\hat{k}}}{n-1}.$$

We can easily prove that $D_{\hat{k}}(\mathcal{T}) = D_{\hat{k}}$ for any $k = 1, ..., n$.

□

Now we examine the case where there are no internal vertices (see Definition 6).

Theorem 10. *Let $n \in \mathbb{N}$, $n \geq 3$ and let $\{D_I\}_{I\in\binom{[n]}{n-1}}$ be a family of positive real numbers.*

There exists a positive-weighted tree $\mathcal{T} = (T, w)$ with exactly n vertices, $1, ..., n$, and such that $D_{\hat{i}}(\mathcal{T}) = D_{\hat{i}}$ for any $i \in [n]$ if and only if the following three conditions hold:

(i)

$$(n-2)D_{\hat{i}} \leq \sum_{j\neq i} D_{\hat{j}} \tag{6}$$

for any $i \in [n]$ and at most one of the inequalities (6) is an equality.

(ii) either one of the inequalities (6) is an equality or the maximum in $\{D_{\hat{i}}\}_{i\in[n]}$ is acheived at least twice.

(iii) the maximum in $\{D_{\hat{i}}\}_{i\in[n]}$ is acheived at most $n-2$ times.

Proof. $\Rightarrow$ (i) The inequality follows from the analogous implication of Theorem 9.

(ii), (iii) Since $n \geq 3$, at least one of the vertices of T must have degree greater or equal than 2. Besides observe that, if a vertex k of T has degree greater or equal than 2, then $D_{\hat{k}}(\mathcal{T}) = D_{1,....,n}(\mathcal{T})$, which is greater or equal than $D_{\hat{j}}(\mathcal{T})$ for every $j = 1, ..., n$. So $D_{\hat{k}}(\mathcal{T})$ is the maximum of $\{D_{\hat{i}}(\mathcal{T})\}_{i\in[n]}$.

Thus, if in T there are at least two vertices of degree greater or equal than 2, then the maximum in $\{D_{\hat{i}}(\mathcal{T})\}_{i\in[n]}$ is acheived twice.

If in T there is only one vertex, k, of degree greater or equal than 2, then T is a star tree with center k and we can check easily that only one of the inequalities (6) is an equality.

Therefore we have proved (ii).

To prove (iii), observe that in T there are at least two leaves, r and s. Since they are leaves, we have:

$$D_{\hat{r}}(\mathcal{T}), D_{\hat{s}}(\mathcal{T}) < D_{1,...,n}(\mathcal{T}) = D_{\hat{k}}(\mathcal{T})$$

for any k vertex of degree at least 2. So the maximum in $\{D_{\hat{i}}(\mathcal{T})\}_{i\in[n]}$ is acheived at most $n-2$ times and we have proved (iii).

$\Leftarrow$ Suppose (i),(ii), and (iii) hold.

- If at least one (and then, by assumption, exactly one) of the inequalities (6) is an equality, let us say $(n-2)D_{\hat{r}} = \sum_{j=1,...,n,\, j\neq r} D_{\hat{j}}$, let $\mathcal{T}$ be the star tree with $\{1, ..., \hat{r}, ..., n\}$ as set of leaves and center r and, for $k = 1, ..., n$, $k \neq r$, let

$$w(e(r,k)) = \frac{\sum_{j=1,...,n,\, j\neq k} D_{\hat{j}} - (n-2)D_{\hat{k}}}{n-1}.$$

  We can easily prove that $D_{\hat{k}}(\mathcal{T}) = D_{\hat{k}}$ for any $k = 1, ..., n$.

- If all the inequalities (6) are strict, then, by assumption, the maximum in $\{D_I\}_{I\in\binom{[n]}{n-1}}$ is acheived at least twice. So we can suppose

$$D_{\hat{1}} = ... = D_{\hat{h}} > D_{\widehat{h+1}}, ..., D_{\hat{n}}$$

  for some $h \geq 2$. By (iii) we have that $n-h \geq 2$. Let us divide the set $\{h+1, ..., n\}$ into two nonempty subsets: $\{h+1, ..., h+s\}$ and $\{h+s+1, ..., n\}$.

  Let $\mathcal{T} = (T, w)$ be the weighted tree with leaves $h+1, ..., n$ in Fig. 1 such that

  $w(e(k,1)) = D_{\hat{1}} - D_{\hat{k}}$ for $k = h+1, ..., h+s$,
  $w(e(k,h)) = D_{\hat{1}} - D_{\hat{k}}$ for $k = h+s+1, ..., n$,
  $w(e(k,k+1)) = \frac{\sum_{j\geq h+1} D_{\hat{j}} - (n-h-1)D_{\hat{1}}}{h-1}$ for $k = 1, ..., h-1$.

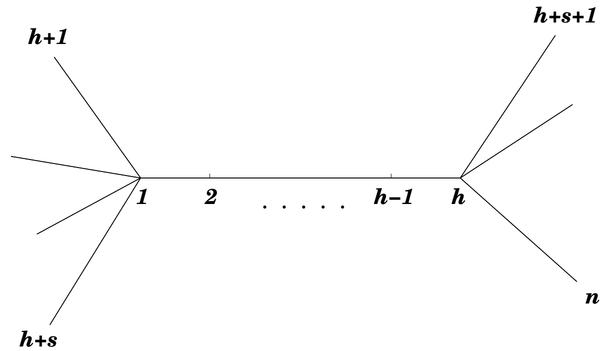

Figure 1: Tree in the case all the inequalities are strict

So the path between 1 and h has weight $\sum_{j \geq h+1} D_{\hat{j}} - (n-h-1) D_{\hat{1}}$. Observe that the weights of the edges of $\mathcal{T}$ are positive, in fact $D_{\hat{1}} > D_{\hat{k}}$ for $k = h+1, ..., n$ and

$$\sum_{j \geq h+1} D_{\hat{j}} - (n-h-1) D_{\hat{1}} = \sum_{j \geq 2} D_{\hat{j}} - (n-2) D_{\hat{1}},$$

which is positive because we are in the case where all the inequalities (6) are strict.

Let $k \in \{1, ..., h\}$. Then $D_{\hat{k}}(\mathcal{T})$ is the sum of the weights of all the edges of $\mathcal{T}$, thus:

$$D_{\hat{k}}(\mathcal{T}) = \sum_{j=h+1,...,n} (D_{\hat{1}} - D_{\hat{j}}) + \sum_{j=h+1,...,n} D_{\hat{j}} - (n-h-1) D_{\hat{1}} = D_{\hat{1}} = D_{\hat{k}}.$$

Let $k \in \{h+1, ..., n\}$. Then $D_{\hat{k}}(\mathcal{T})$ is the sum of the weights of all the edges of $\mathcal{T}$ but the edge $e(k,1)$ if $k \in \{h+1, ..., h+s\}$ or the edge $e(k,h)$ if $k \in \{h+s+1, ..., n\}$. Hence

$$D_{\hat{k}}(\mathcal{T}) = D_{\hat{1}} - (D_{\hat{1}} - D_{\hat{k}}) = D_{\hat{k}}.$$

□

4 $(n-1)$-dissimilarity vectors of graphs with n vertices

In this section we want to examine when a family of positive real numbers $\{D_I\}_{I \in \binom{[n]}{n-1}}$ is graphlike. First we consider the case of graphs with exactly n vertices.

Theorem 11. *Let $n \in \mathbb{N},\ n \geq 3$. Let $\{D_I\}_{I \in \binom{[n]}{n-1}}$ be a family of positive real numbers.*

There exists a positive weighted graph $\mathcal{G} = (G, w)$ with exactly n vertices, $1, ..., n$, and with $D_{\hat{i}}(\mathcal{G}) = D_{\hat{i}}$ for any $i = 1, ..., n$ if and only if the following two conditions hold:

(i)

$$(n-2) D_{\hat{i}} \leq \sum_{j=1,...,n,\ j \neq i} D_{\hat{j}} \tag{7}$$

for any $i \in [n]$,

(ii) if the maximum in $\{D_{\hat{i}}\}_{i\in[n]}$ is acheived at least twice, the inequalities (7) are strict.

Remark 12. *Condition (i) implies that, for any $k \in \mathbb{N}$ with $1 \leq k \leq n-2$,*

$$kD_{\hat{i}} \leq \sum_{j\in\{i_1,....,i_{k+1}\}} D_{\hat{j}} \tag{8}$$

for any distinct $i, i_1, ..., i_{k+1} \in [n]$, in particular condition (i) implies the triangle inequalities.

Proof. Obviously we can suppose that, in (8), $D_{\hat{i}} = max_{j\in[n]} D_{\hat{j}}$. Therefore

$$(n-k-2)D_{\hat{i}} \geq \sum_{j\in[n]-\{i,i_1,....,i_{k+1}\}} D_{\hat{j}}.$$

The inequality above and condition (i) imply at once the inequality (8). □

Proof of Theorem 11 ⇒ We can suppose $i = 1$ in (7), so the inequality we have to prove becomes

$$(n-2)D_{\hat{1}} \leq \sum_{j=2,...,n} D_{\hat{j}}.$$

Let H be a subtree of G realizing $D_{\hat{n}}$. Observe that we can construct an injective map

$$\varepsilon : V(H) - \{1\} \longrightarrow E(H)$$

sending a vertex v to an edge incident with v (consider H as rooted tree with 1 as root and send any leaf to the unique incident edge, then delete these edges and repeat the procedure until you arrive at the root).

Observe that

$$D_{\hat{1}} \leq D_{\hat{i}} + w(\varepsilon(i))$$

for $i = 2, ..., n-1$, in fact: let R_i be the subgraph given by the union of a subtree realizing $D_{\hat{i}}$ and of $\varepsilon(i)$; the subgraph R_i is connected (because the ends of $\varepsilon(i)$ are i and a vertex among $1, ..., n$ different from i, thus a vertex of the subtree realizing $D_{\hat{i}}$); besides $2, ..., n \in V(R_i)$; hence $D_{\hat{1}} \leq w(R_i) = D_{\hat{i}} + w(\varepsilon(i))$. Therefore

$$(n-2)D_{\hat{1}} \leq \sum_{i=2,...,n-1} \big(D_{\hat{i}} + w(\varepsilon(i))\big) \leq$$

$$\leq \sum_{i=2,...,n-1} D_{\hat{i}} + \sum_{i=2,...,n-1} w(\varepsilon(i)) \leq \sum_{i=2,...,n-1} D_{\hat{i}} + D_{\hat{n}} = \sum_{i=2,...,n} D_{\hat{i}}.$$

Suppose now that the maximum of $\{D_{\hat{i}}\}_{i\in[n]}$ is achieved at least twice. We want to show that the inequalities (7) are strict.

We can suppose $D_{\hat{1}} = D_{\hat{2}} \geq D_{\hat{j}}$ for $j = 3, ..., n$. Obviously, to prove that the inequalities (7) are strict, it suffices to prove that

$$(n-2)D_{\hat{1}} < \sum_{i=2,...,n} D_{\hat{i}}.$$

We have already proved that $D_{\hat{1}} \leq D_{\hat{i}} + w(\varepsilon(i))$ for $i = 2, ..., n-1$, in particular for $i = 3, ..., n-1$; besides we know that $D_{\hat{1}} = D_{\hat{2}}$. Thus we get:

$$(n-2)D_{\hat{1}} \;\leq\; D_{\hat{2}} + \sum_{i=3,...,n-1} \big(D_{\hat{i}} + w(\varepsilon(i))\big) \;=\; \sum_{i=2,...,n-1} D_{\hat{i}} + \sum_{i=3,...,n-1} w(\varepsilon(i)) \;<$$

$$< \sum_{i=2,...,n-1} D_{\hat{i}} + \sum_{i=2,...,n-1} w(\varepsilon(i)) \;\leq\; \sum_{i=2,...,n-1} D_{\hat{i}} + D_{\hat{n}} = \sum_{i=2,...,n} D_{\hat{i}}.$$

$\Leftarrow$ Let $n = 3$. Let $\mathcal{G}$ be the complete graph with vertices $1, 2, 3$ and weights $w(e(1,2)) = D_{\hat{3}}$, $w(e(1,3)) = D_{\hat{2}}$, $w(e(2,3)) = D_{\hat{1}}$. Obviously $D_{\hat{i}}(\mathcal{G}) = D_{\hat{i}}$ for $i = 1, 2, 3$.

Let $n \geq 4$. We consider two cases:

1) the maximum in $\{D_{\hat{i}}\}_{i \in [n]}$ is acheived at least twice,

2) the maximum in $\{D_{\hat{i}}\}_{i \in [n]}$ is acheived only once.

1) Suppose $D_{\hat{1}} = ... = D_{\hat{k}} > D_{\widehat{k+1}}, ..., D_{\hat{n}}$ for some $k \geq 2$. Let

$$a = \frac{D_{\widehat{k+1}} + ... + D_{\hat{n}} - (n-k-1)D_{\hat{1}}}{n-2}$$

and, for any $i = k+1, ..., n$, let

$$x_i = \frac{D_{\widehat{k+1}} + ... + D_{\hat{n}}}{n-2} + \frac{k-1}{n-2} D_{\hat{1}} - D_{\hat{i}}.$$

We can easily prove that

$$a \leq x_i$$

for any $i = k+1, ..., n$. Besides observe that a is positive by assumptions (i) and (ii) (and then also the x_i are positive).

Let $\mathcal{G}$ be the weighted graph defined in the following way: consider the complete graph with vertices $1, ..., k$ and weights of the edges equal to a and then, for any $i = k+1, ..., n$, draw an edge joining i and 1 and an edge joining i and k, both with weight x_i.

Since $a \leq x_i$ for any $i = k+1, ..., n$, we get:

$$D_{\hat{1}}(\mathcal{G}) = ... = D_{\hat{k}}(\mathcal{G}) = (k-2)a + x_{k+1} + ... + x_n = D_{\hat{1}} = ... = D_{\hat{k}}$$

and, for any $i = k+1, ..., n$, we have:

$$D_{\hat{i}}(\mathcal{G}) = (k-1)a + \sum_{j=k+1,...,n,\; j \neq i} x_j = D_{\hat{i}}.$$

2) We prove the statement by induction on n. Precisely we prove, by induction on n (with $n = 4$ as base case), that if (i) holds and the maximum in $\{D_{\hat{i}}\}_{i \in [n]}$ is acheived only once, then there exists a weighted graph $\mathcal{G} = (G, w)$ with exactly n vertices such that:

- $D_{\hat{j}} = D_{\hat{j}}(\mathcal{G})$ for any $j = 1, ..., n$
- if $D_{\hat{i}}(\mathcal{G})$ is the maximum in $\{D_{\hat{j}}\}_{j\in[n]}$, then any subgraph realizing $D_{\hat{i}}(\mathcal{G})$ has necessarily i as vertex, so in particular $D_{1,...,n}(\mathcal{G}) = D_{\hat{i}}(\mathcal{G})$.

Let $n = 4$. Suppose that $D_{\hat{1}} > D_{\hat{2}}, D_{\hat{3}}, D_{\hat{4}}$. Without loss of generality we can also suppose that $D_{\hat{3}} \geq D_{\hat{2}}$. Let $\mathcal{G}$ be the weighted graph shown in Figure 2.

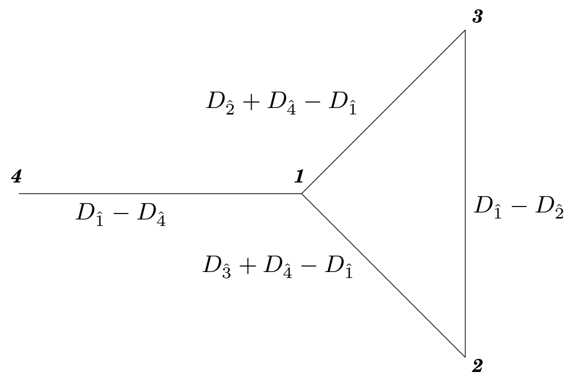

Figure 2: Graph with 3-dissimilarity vector $(D_{\hat{1}}, D_{\hat{2}}, D_{\hat{3}}, D_{\hat{4}})$

Observe that it is positive weighted, in fact: obviously $D_{\hat{1}} - D_{\hat{4}} > 0$ and $D_{\hat{1}} - D_{\hat{2}} > 0$; besides

$$D_{\hat{3}} + D_{\hat{4}} - D_{\hat{1}} > 0,$$

because $2D_{\hat{1}} \leq D_{\hat{2}} + D_{\hat{3}} + D_{\hat{4}}$ by (7) and $D_{\hat{1}} > D_{\hat{2}}$; analogously

$$D_{\hat{2}} + D_{\hat{4}} - D_{\hat{1}} > 0.$$

Furthermore we can see easily that:
$w(e(2,3)) \leq w(e(1,2))$,
$w(e(1,3)) \leq w(e(1,2))$,
$w(e(1,3)) + w(e(2,3)) \geq w(e(1,2))$,
$w(e(1,2)) + w(e(2,3)) \geq w(e(1,3))$.
Thus we get:
$D_{\hat{1}}(\mathcal{G}) = w(e(1,4)) + w(e(1,3)) + w(e(2,3)) = D_{\hat{1}}$,
$D_{\hat{2}}(\mathcal{G}) = w(e(1,4)) + w(e(1,3)) = D_{\hat{2}}$,
$D_{\hat{3}}(\mathcal{G}) = w(e(1,4)) + w(e(1,2)) = D_{\hat{3}}$,
$D_{\hat{4}}(\mathcal{G}) = w(e(1,3)) + w(e(2,3)) = D_{\hat{4}}$.
Now we want to prove the induction step. Let $n \geq 5$. Without loss of generality we can suppose that

$$D_{\hat{1}} > D_{\hat{n}} \geq D_{\hat{j}}$$

for any $j = 2, ..., n-1$.

Let $x = D_{\hat{1}} - D_{\hat{n}}$ and define $\tilde{D}_{1,...,\hat{i},....,n-1}$ ($\tilde{D}_{\hat{i}}$ for short) for $i = 1, ..., n-1$ in the following way:

$$\tilde{D}_{\hat{i}} = \begin{cases} D_{\hat{n}} & \text{for } i = 1 \\ D_{\hat{i}} - x & \text{for } i = 2, ..., n-1 \end{cases}$$

Observe that the $\tilde{D}_{\hat{i}}$ are positive, in fact the inequality

$$(n-2)D_{\hat{1}} \leq \sum_{j=2,...,n} D_{\hat{j}}$$

(which follows from (i)) and the inequalities

$$D_{\hat{1}} > D_{\hat{j}}$$

for any $j = 2, ..., n$ (in particular for $j \neq 1, i, n$) imply that

$$D_{\hat{1}} < D_{\hat{n}} + D_{\hat{i}}.$$

Observe also that $\tilde{D}_{\hat{1}} > \tilde{D}_{\hat{i}}$ for $i = 2, ..., n-1$. Therefore also in the set $\{\tilde{D}_{\hat{i}}\}_{i \in [n-1]}$, the maximum is acheived only once (by $\tilde{D}_{\hat{1}}$). Besides the $\tilde{D}_{\hat{i}}$ for $i = 1, ..., n-1$ satisfy (7) with $n-1$ instead of n, in fact:

obviously it suffices to prove (7) when the first member is the maximum, that is $(n-2)\tilde{D}_{\hat{1}}$, so it suffices to prove that

$$(n-3)\tilde{D}_{\hat{1}} \leq \sum_{j=2,...,n-1} \tilde{D}_{\hat{j}},$$

which is equivalent to

$$(n-3)D_{\hat{n}} \leq \sum_{j=2,...,n-1} D_{\hat{j}} - (n-2)D_{\hat{1}} + (n-2)D_{\hat{n}},$$

that is

$$(n-2)D_{\hat{1}} \leq \sum_{j=2,...,n-1} D_{\hat{j}} + D_{\hat{n}},$$

which follows from (7).

Therefore, by induction assumption, there exists a weighted graph $\tilde{\mathcal{G}} = (\tilde{G}, \tilde{w})$ with vertices $1, ..., n-1$ such that: $D_{\hat{i}}(\tilde{\mathcal{G}}) = \tilde{D}_{\hat{i}}$ for any $i = 1, ..., n-1$ and any subgraph realizing $D_{\hat{1}}(\tilde{\mathcal{G}})$ (which is the maximum of the $D_{\hat{i}}(\tilde{\mathcal{G}})$) has 1 as vertex (so $D_{\hat{1}}(\tilde{\mathcal{G}})$ is equal to $D_{1,...,n-1}(\tilde{\mathcal{G}})$). Let $\mathcal{G}$ be the graph obtained from $\tilde{\mathcal{G}}$ by adding an edge E incident with 1 with weight x; call n the other end of E.

Observe that any subgraph realizing $D_{\hat{1}}(\mathcal{G})$ has 1 as vertex by the construction of $\mathcal{G}$. We want to show that $D_{\hat{i}}(\mathcal{G}) = D_{\hat{i}}$ for any $i = 1, ..., n$. Obviously,

$$D_{\hat{n}}(\mathcal{G}) = D_{1,....,n-1}(\tilde{\mathcal{G}}) = D_{\hat{1}}(\tilde{\mathcal{G}}) = \tilde{D}_{\hat{1}} = D_{\hat{n}},$$

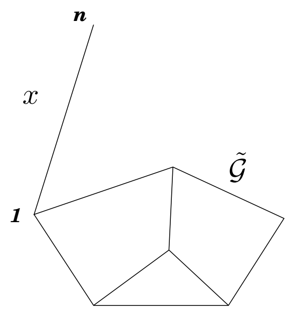

Figure 3: $\mathcal{G}$ and $\tilde{\mathcal{G}}$.

$$D_{\hat{1}}(\mathcal{G}) = x + D_{1,....,n-1}(\tilde{\mathcal{G}}) = x + D_{\hat{1}}(\tilde{\mathcal{G}}) = x + \tilde{D}_{\hat{1}} = D_{\hat{1}}.$$

Besides, for $i = 2, ..., n-1$,

$$D_{\hat{i}}(\mathcal{G}) = x + D_{\hat{i}}(\tilde{\mathcal{G}}) = x + \tilde{D}_{\hat{i}} = x + D_{\hat{i}} - x = D_{\hat{i}}.$$

□

The case of graphs with internal vertices is more difficult: in this case condition (7) is not necessary: see Figure 4 for an example of a graph with four external vertices such that the 3-dissimilarity vector doesn't satisfy condition (7). Here we study the case with internal vertices only in the case $n = 4$. It seems difficult to generalize the result to n greater than 4.

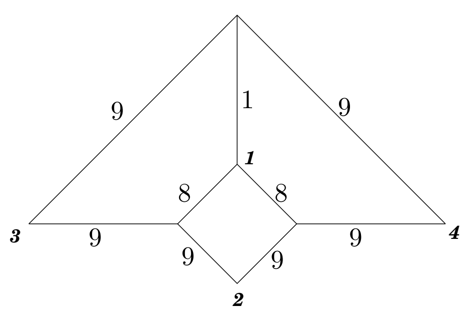

Figure 4: Example of weighted graph such that $2D_{\hat{1}} > D_{\hat{4}} + D_{\hat{3}} + D_{\hat{2}}$.

Theorem 13. *Let $D_{1,2,3}, D_{1,2,4}, D_{1,3,4}, D_{2,3,4} \in \mathbb{R}_+$; as usual we will denote them respectively by $D_{\hat{4}}, D_{\hat{3}}, D_{\hat{2}}, D_{\hat{1}}$. There exists a weighted graph $\mathcal{G} = (G, w)$ with $[4]$ subset of $V(G)$ such that $D_{\hat{i}}(\mathcal{G}) = D_{\hat{i}}$ for $i = 1, 2, 3, 4$ if and only if*

(i)

$$5D_{\hat{t}} \leq 3D_{\hat{k}} + 3D_{\hat{j}} + 2D_{\hat{i}}$$

for any distinct $i, j, k, t \in [4]$,

(ii)

$$D_{\hat{i}} < D_{\hat{k}} + D_{\hat{j}}$$

for any distinct $i, j, k \in [4]$.

Remark 14. *Condition (i) implies the triangle inequalities (that is the inequalities $D_{\hat{i}} \leq D_{\hat{j}} + D_{\hat{k}}$ for any i, j, k distinct in $[4]$), but not the strict triangle inequalities.*

Proof. Condition (i) implies

$$D_{\hat{t}} \leq \frac{3}{5} D_{\hat{k}} + \frac{3}{5} D_{\hat{j}} + \frac{2}{5} D_{\hat{i}}$$

for any distinct $i, j, k, t \in [4]$, so we get:

$$\begin{aligned} 5D_{\hat{t}} &\leq 3D_{\hat{k}} + 3D_{\hat{j}} + 2D_{\hat{i}} \leq \\ &\leq 3D_{\hat{k}} + 3D_{\hat{j}} + 2\left(\frac{3}{5} D_{\hat{k}} + \frac{3}{5} D_{\hat{j}} + \frac{2}{5} D_{\hat{t}}\right) = \\ &= \frac{21}{5} D_{\hat{k}} + \frac{21}{5} D_{\hat{j}} + \frac{4}{5} D_{\hat{t}}, \end{aligned}$$

hence

$$\frac{21}{5} D_{\hat{t}} \leq \frac{21}{5} D_{\hat{k}} + \frac{21}{5} D_{\hat{j}}.$$

Obviously condition (i) does not imply the strict triangle inequalities: in fact, if we take $D_{\hat{4}} = D_{\hat{3}} = D_{\hat{1}} + D_{\hat{2}}$, condition (i) is satisified. $\square$

Proof of Theorem 13. $\Rightarrow$ Let $\mathcal{G} = (G, w)$ be a weighted graph and let $[4] \subset V(G)$. Let $D_{\hat{t}}(\mathcal{G}) = D_{\hat{t}}$ for any distinct $t \in [4]$. The subgraph realizing $D_{\hat{t}}(\mathcal{G})$ is necessarily a tree with two or three leaves. For any $t \in [4]$, we choose a subtree realizing $D_{\hat{t}}(\mathcal{G})$.

We call a_1, a_2, a_3 the weights of the branches of the subtree realizing $D_{\hat{4}}(\mathcal{G})$ if it is a tree with three leaves, $1, 2, 3$. If it is a tree with two leaves, for instance if it is a tree with leaves 1 and 3, we call a_1 the weight of the path between 1 and 2, a_3 the weight of the path between 2 and 3 and we set $a_2 = 0$ and analogously in the other cases (see Figure 5).

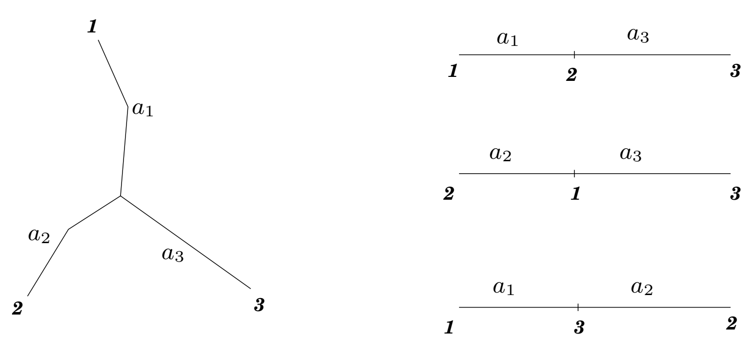

Figure 5: a_1, a_2, a_3

In an analogous way we call b_1, b_2, b_4 the weights of the branches of the subtree realizing $D_{\hat{3}}(\mathcal{G})$, we call c_1, c_3, c_4 the weights of the branches of the subtree realizing $D_{\hat{2}}(\mathcal{G})$, and, finally, we call d_2, d_3, d_4 the weights of the branches of the subtree realizing $D_{\hat{1}}(\mathcal{G})$.

To prove (i), up to permuting $1,2,3,4$, we can suppose $t=1, k=4, j=3, i=2$, so we have to prove that

$$5D_{\hat{1}} \leq 3D_{\hat{4}} + 3D_{\hat{3}} + 2D_{\hat{2}}.$$

Up to swapping the vertices 4 and 3, we can suppose $b_1 \leq a_1$; thus we have:

$$\begin{aligned}
5D_{\hat{1}} \leq (D_{\hat{4}} + b_1 + b_4) + (D_{\hat{4}} + b_1 + b_4) + (D_{\hat{3}} - b_1 + a_2 + a_3) + \\
+(D_{\hat{2}} + b_1 + b_2) + (D_{\hat{2}} + b_1 + b_2) = \\
= 2D_{\hat{4}} + D_{\hat{3}} + 2D_{\hat{2}} + (3b_1 + 2b_2 + 2b_4 + a_2 + a_3) \leq \\
\leq 2D_{\hat{4}} + D_{\hat{3}} + 2D_{\hat{2}} + (2b_1 + 2b_2 + 2b_4 + a_1 + a_2 + a_3) = \\
= 3D_{\hat{4}} + 3D_{\hat{3}} + 2D_{\hat{2}};
\end{aligned}$$

Observe that all the inequalities hold also if some of the a_i or some of the b_i is zero. So we have proved (i).

To prove (ii), up to permuting $1,2,3,4$, we can suppose $i=4, k=1, j=2$. So we have to prove that

$$D_{\hat{4}} < D_{\hat{1}} + D_{\hat{2}}.$$

If both the tree realizing $D_{\hat{1}}$ and the tree realizing $D_{\hat{2}}$ have three leaves, we get:

$$D_{\hat{4}} \leq d_2 + d_3 + c_3 + c_1 < D_{\hat{1}} + D_{\hat{2}}.$$

If the tree realizing $D_{\hat{1}}$ has three leaves and the tree realizing $D_{\hat{2}}$ has two leaves, we get:

$$D_{\hat{4}} \leq d_2 + d_3 + c_3 + c_1 < D_{\hat{1}} + D_{\hat{2}}$$

if the leaves of the tree realizing $D_{\hat{2}}$ are $1,3$,

$$D_{\hat{4}} \leq d_2 + d_3 + c_3 < D_{\hat{1}} + D_{\hat{2}}$$

if the leaves of the tree realizing $D_{\hat{2}}$ are $4,3$,

$$D_{\hat{4}} \leq d_2 + d_3 + c_1 < D_{\hat{1}} + D_{\hat{2}}$$

if the leaves of the tree realizing $D_{\hat{2}}$ are $1,4$.

Analogously we can argue if the tree realizing $D_{\hat{1}}$ has two leaves and the tree realizing $D_{\hat{2}}$ has three leaves.

Finally, if both the tree realizing $D_{\hat{1}}$ and the tree realizing $D_{\hat{2}}$ have two leaves, we get:

$$D_{\hat{4}} \leq d_2 + d_3 + c_1 < D_{\hat{1}} + D_{\hat{2}}$$

if the leaves of the tree realizing $D_{\hat{2}}$ are $1,3$ and the leaves of the tree realizing $D_{\hat{1}}$ are $2,3$ and analogously we can argue in the other cases.

$\Leftarrow$ We can suppose $D_{\hat{4}} \geq D_{\hat{3}} \geq D_{\hat{2}} \geq D_{\hat{1}}$. Let $\mathcal{G} = (G, w)$ be the weighted graph in Figure 6, where:

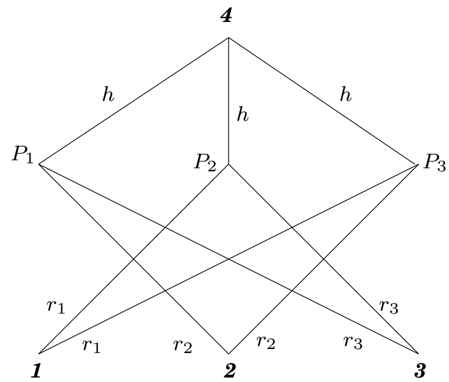

Figure 6: A graph realizing $(D_{\hat{1}}, D_{\hat{2}}, D_{\hat{3}}, D_{\hat{4}})$.

$h := \frac{D_{\hat{1}}+D_{\hat{2}}-D_{\hat{4}}}{2}$,

$r_1 := \frac{D_{\hat{4}}+D_{\hat{2}}+2D_{\hat{3}}-3D_{\hat{1}}}{4}$,

$r_2 := \frac{D_{\hat{4}}+D_{\hat{1}}+2D_{\hat{3}}-3D_{\hat{2}}}{4}$,

$r_3 := \frac{D_{\hat{4}}+D_{\hat{1}}+D_{\hat{2}}-2D_{\hat{3}}}{4}$,

that is, G is a graph with vertices $1, 2, 3, 4, P_1, P_2, P_3$ and, for any $i \in [3]$, we join the vertices 4 and P_i with an edge of weight h and, for any $i \in [3], j \in [3] - \{i\}$, we join the vertices i and P_j with an edge of weight r_i.

From assumption (ii) and from the fact that $D_{\hat{4}} \geq D_{\hat{3}} \geq D_{\hat{2}} \geq D_{\hat{1}}$, we get easily that h, r_1, r_2, r_3 are positive. Besides observe that $2h \geq r_3$ (by condition (i)), hence:

$D_{\hat{1}}(\mathcal{G}) = h + r_2 + r_3 = D_{\hat{1}}$,

$D_{\hat{2}}(\mathcal{G}) = h + r_1 + r_3 = D_{\hat{2}}$,

$D_{\hat{3}}(\mathcal{G}) = h + r_1 + r_2 = D_{\hat{3}}$,

$D_{\hat{4}}(\mathcal{G}) = r_1 + r_2 + 2r_3 = D_{\hat{4}}$.

□

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